Abstract Submitted
for the DPP11 Meeting of
The American Physical Society

The Kinetic Theory Molecular Dynamics Method CHRIS FICHTL, MICHAEL MURILLO, LANL, FRANK GRAZIANI, LLNL, CIMARRON COLLABORATION — We are interested in simulating plasmas under thermonuclear burn conditions relevant to NIF. As such, we have recently developed the Kinetic Theory Molecular Dynamics (KTMD) method, which takes advantage of the fact that the plasma electrons are typically moderately degenerate and weakly coupled, whereas the ions are classical and moderately to strongly coupled. The basic approach of KTMD is to describe the fully non-equilibrium electron dynamics with an appropriate kinetic equation while leaving the ion dynamics to MD. The current version of KTMD self-consistently follows the time evolution of a Fermi gas via the time-dependent, fully nonlinear Wigner-Poisson system. Our approach, its associated implementation, and preliminary physics benchmarking results, such as nonlinear plasma waves and instabilities, will be presented. We describe a Langevin approach designed to mitigate numerical errors causing the Fermi distribution to relax towards a Maxwellian during long simulations. Ideas for extending the current capability, such as extending the mean-field approach by including collisions and quantum mechanical smearing, will be outlined.

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Date submitted: 14 Jul 2011 Electronic form version 1.4